Perturbation theory of von Neumann Entropy

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Abstract

In quantum information theory, von Neumann entropy plays an important role. The entropies can be obtained analytically only for a few states. In continuous variable system, even evaluating entropy numerically is not an easy task since the dimension is infinite. We develop the perturbation theory systematically for calculating von Neumann entropy of non-degenerate systems as well as degenerate systems. The result turns out to be a practical way of the expansion calculation of von Neumann entropy.

1 Introduction

In quantum information theory, von Neumann entropy of a state appears in many basic theorems such as quantum source coding [1], quantum channel coding of classical information [2] [3], quantum channel coding of quantum information [4] [5]. The later two are problems of channel capacities, which are maxima of Holevo quantity and coherent information, respectively (usually the regulation procedure should be taken). The problems can be reduced to the calculation of von Neumann entropy. The basic method to obtain the von Neumann entropy of a state is to calculate its spectrum. The spectrum can seldom be obtained for a given state. Meanwhile numeric calculation of the spectrum may encounter problems for continuous variable system which has an infinite dimensional Hilbert space. Hence a perturbation theory for the von Neumann entropy of a state is needed. While quantum mechanics provides us the theory of lower order perturbation to the energy levels, here we will develop a systematical theory of the entropy perturbation up to any order of precision.

2 The perturbation to the entropy of a non-degenerate system

2.1 The perturbation of entropy via eigenvalues

A non-degenerate quantum system is a density matrix ρ_0 with its eigenvalues $E_n \neq E_m$ for all $n \neq m$, where n (or m) is the number (or vector number) specifying the quantum eigenstate. The usual quantum perturbation theory for the non-degenerate systems gives the first and second order eigenvalue perturbations

$$E_n^{(1)} = H_{nn}, \tag{1}$$

$$E_n^{(2)} = \sum_{m\neq n} \frac{|H_{nm}|^2}{E_n - E_m}, \tag{2}$$

when the perturbation to the density matrix is the matrix H, where $H_{nm} = \langle\psi_n| H |\psi_m\rangle$, with $|\psi_n\rangle$ the eigenvector of the density operator ρ_0 corresponding to the eigenvalue E_n . As usual, the perturbed density matrix can be written as $\rho = \rho_0 + \varepsilon H$. Since ρ and ρ_0 are density matrices, we have $H^\dagger = H$,and $TrH = 0$. Thus we have $\sum_n E_n^{(1)} = 0$,and it is clear that $\sum_n E_n^{(2)} = 0$. The total eigenvalue up to the second order is $E_n^{(t)} = E_n + \varepsilon E_n^{(1)} + \varepsilon^2 E_n^{(2)}$. The entropy of the state up to the second order perturbation is $S(\rho) = -Tr\rho\log\rho = -\sum_n E_n^{(t)} \log E_n^{(t)} + o(\varepsilon^2)$. Thus we have $S(\rho) = S(\rho_0) + \varepsilon\frac{dS(\rho_0)}{d\varepsilon} + \frac{1}{2}\varepsilon^2\frac{d^2S(\rho_0)}{d\varepsilon^2} + o(\varepsilon^2)$ with

$$\frac{dS(\rho_0)}{d\varepsilon} = -\sum_n H_{nn}\log E_n \tag{3}$$

$$\frac{d^2S(\rho_0)}{d\varepsilon^2} = -\sum_n \frac{H_{nn}^2}{E_n} - 2\sum_n E_n^{(2)}\log E_n \tag{4}$$

2.2 The expansion formula of the entropy

For $a>0$, we have $\log a=\int_0^\infty \frac{at-1}{a+t}\frac{dt}{1+t^2}$. Similarly, for a positive operator A, we have $\log A=\int_0^\infty \frac{At-1}{A+t}\frac{dt}{1+t^2}$.[6] Thus $\log A-\log B=-\lim_{M\to\infty}\int_0^M(\frac{1}{A+t}-\frac{1}{B+t})dt$ for positive operators A and B. $\frac{dS(\rho_0)}{d\varepsilon}=-\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}Tr[\rho\log\rho-\rho_0\log\rho_0]=-\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}Tr[\rho_0(\log\rho-\log\rho_0)]-Tr[H\log\rho_0]$, Note that $\frac{1}{A+t}=\frac{1}{t}\sum_{k=0}^{\infty}(-1)^k(\frac{A}{t})^k$, we have

$$\frac{dS(\rho_0)}{d\varepsilon}=\int_0^\infty Tr\{\rho_0(\rho_0+t)^{-1}H(\rho_0+t)^{-1}\}dt-Tr[H\log\rho_0]. \tag{5}$$

Evaluating in the eigenbasis of ρ_0, it reads

$$\begin{aligned}\frac{dS(\rho_0)}{d\varepsilon} &= \sum_n\int_0^\infty E_n(E_n+t)^{-2}H_{nn}dt-\sum_n H_{nn}\log E_n\\ &= -\sum_n H_{nn}\log E_n,\end{aligned} \tag{6}$$

where $TrH=0$ has been used. It coincides with Eq.(3), the result derived from the perturbation of the eigenvalues.

The second derivative of the entropy at ρ_0 is $\frac{d^2S(\rho_0)}{d\varepsilon^2}=-\lim_{\varepsilon\to 0}\frac{1}{\varepsilon^2}Tr[\rho_+\log\rho_++\rho_-\log\rho_--2\rho_0\log\rho_0]$, where $\rho_\pm=\rho_0\pm\varepsilon H$. The derivative can be rewritten as P_1+P_2, the two parts are $P_1=-\lim_{\varepsilon\to 0}\frac{1}{\varepsilon^2}Tr\rho_0(\log\rho_++\log\rho_--2\log\rho_0)=2\int_0^\infty Tr\rho_0(\rho_0+t)^{-1}H\ (\rho_0+t)^{-1}H(\rho_0+t)^{-1}dt$ and $P_2=-\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}TrH(\log\rho_+-\log\rho_-)=-2\int_0^\infty TrH(\rho_0+t)^{-1}H(\rho_0+t)^{-1}dt$. With the eigenbasis of ρ_0, we have

$$\begin{aligned}\frac{d^2S(\rho_0)}{d\varepsilon^2} &= -2\sum_{n,m}\int_0^\infty\frac{t\,|H_{nm}|^2}{(E_n+t)^2(E_m+t)}dt\\ &= -\sum_n\frac{|H_{nn}|^2}{E_n}-2\sum_{n,m\neq n}\frac{|H_{nm}|^2E_m}{(E_n-E_m)^2}\log\frac{E_m}{E_n}\\ &= -\sum_n\frac{|H_{nn}|^2}{E_n}-2\sum_{n,m\neq n}\frac{|H_{nm}|^2}{E_n-E_m}\log E_n\end{aligned} \tag{7}$$

Note that Eq.(4) and Eq. (7) are strictly the same, and the non-degenerate condition is used.

The n^{th} derivative of the entropy can also be carried out. From the definition of the derivative, we have $\frac{d^nS(\rho_0)}{d\varepsilon^n}=-\lim_{\varepsilon\to 0}\frac{1}{\varepsilon^n}\sum_{l=0}^n S(\rho_0+l\varepsilon)\binom{l}{n}(-1)^l=P_3+P_4$, with $P_3=-\lim_{\varepsilon\to 0}\frac{1}{\varepsilon^n}\sum_{l=0}^n Tr\rho_0\log(\rho_0+l\varepsilon)\binom{l}{n}(-1)^l=n!\int_0^\infty Tr\rho_0(\rho_0+t)^{-1}[H(\rho_0+t)^{-1}]^n\ dt$ for $n>0$. $P_4=-\lim_{\varepsilon\to 0}\frac{1}{\varepsilon^n}\sum_{l=0}^n Tr[\varepsilon lH\log(\rho_0+l\varepsilon)]\binom{l}{n}(-1)^l=-n!\int_0^\infty Tr[H(\rho_0+t)^{-1}]^n\ dt$ for $n>1$ (see Appendix A). Thus we have

$$\frac{d^nS(\rho_0)}{d\varepsilon^n}=-(-1)^n n!\int_0^\infty Tr\{t(\rho_0+t)^{-1}[H(\rho_0+t)^{-1}]^n\}dt. \tag{8}$$

The Taylor expansion formula for the entropy of a state $\rho=\rho_0+\varepsilon H$ will be

$$\begin{aligned}S(\rho) &= \sum_{n=0}^{\infty}\frac{\varepsilon^n}{n!}\frac{d^nS(\rho_0)}{d\varepsilon^n}\\ &= S(\rho_0)-\varepsilon Tr[H\log\rho_0]-\sum_{n=2}^{\infty}(-\varepsilon)^n\int_0^\infty Tr\{t(\rho_0+t)^{-1}[H(\rho_0+t)^{-1}]^n\}dt.\end{aligned} \tag{9}$$

We calculate the third and the fourth order perturbation for the case of $H_{nn}=0$, the entropy up to fourth order perturbation is

$$S(\rho)=S(\rho_0)-\varepsilon^2\sum_{n,m\neq n}\frac{|H_{nm}|^2}{E_n-E_m}\log E_n+\varepsilon^3Q_3-\varepsilon^4(Q_{41}+Q_{42}+Q_{43})+o(\varepsilon^4) \tag{10}$$

where Q_3,Q_{41},Q_{42} and Q_{43} are given in Appendix B.

2.3 Perturbation to the one-mode thermal state

Assuming that a one-mode thermal state is perturbed, the perturbed characteristic function is

$$\chi(\mu) = \chi_T(\mu)[1 + \varepsilon(\alpha^*\mu - \alpha\mu^*)], \tag{11}$$

where $\chi_T(\mu) = \exp[-(N + \frac{1}{2}) |\mu|^2]$ is the characteristic function of the one-mode thermal state, with N the average photon number of the state. The density operator can be obtained with $\rho = \int \frac{d^2\mu}{\pi} \chi(\mu) D(-\mu)$, where $D(\mu) = \exp[\mu a^\dagger - \mu^* a]$ is the displacement operator, $a^\dagger$and a are the creation and annihilation operator of the system, respectively. By the method of integral within ordered product operator, the perturbed density operator is

$$\rho = \rho_T + \varepsilon(1 - v)(\alpha a^\dagger \rho_T + \alpha^* \rho_T a). \tag{12}$$

where $\rho_T = (1 - v) \sum_{n=0}^{\infty} v^n |n\rangle \langle n|$ is the unperturbed one-mode thermal state with $v = N/(N + 1)$. It is clear that in the eigenbasis of ρ_T the diagonal elements of the perturbation $H = (1 - v)(\alpha a^\dagger \rho_T + \alpha^* \rho_T a)$ is null, thus in the evaluation of Eq.(9) we only need to consider the off-diagonal elements of H. Evaluating Eq. (9) in the basis of ρ_T,up to ε^4, for a null-diagonal H, the entropy will be

$$S(\rho) = S(\rho_T) - \varepsilon^2 \sum_{n,m\neq n} \frac{|H_{nm}|^2}{E_n - E_m} \log E_n + \varepsilon^3 Q_3 - \varepsilon^4 (Q_{41} + Q_{42} + Q_{43}) + o(\varepsilon^4) \tag{13}$$

In our case, $H_{nm} = (1 - v)(\alpha\sqrt{n} E_{n-1} \delta_{n,m+1} + \alpha^* E_n \sqrt{n+1} \delta_{n,m-1})$. Thus $Q_3 = Q_{41} = 0$ due to the structure of H, and $Q_{43} = |\alpha|^4 [\frac{(1+v)^2}{2v} + \frac{1+v}{1-v} \log v]$, $Q_{42} = -2 |\alpha|^4 [1 + \frac{1+v^2}{1-v^2} \log v]$. The entropy of the perturbed state is

$$S(\rho) = S(\rho_T) - 2\varepsilon^2 |\alpha|^2 \log \frac{1}{v} - \varepsilon^4 |\alpha|^4 [\frac{(1 - v)^2}{2v} + \frac{1 - v}{1 + v} \log \frac{1}{v}] + o(\varepsilon^4). \tag{14}$$

3 The perturbation to the entropy of a degenerate system

3.1 The entropy perturbation up to second order

Note that Eq.(9) is an overall result regardless of the eigenvalue structure of the state ρ_0. The difference between the degenerate system and non-degenerate system comes when we evaluate the entropy. We now classify the eigenvectors according to the eigenvalues of ρ_0. Suppose the eigenvalue E_n correspond to the eigenvector set $\{|n, n_i\rangle, |i = 1, \ldots n_d\}$, these eigenvectors span the subspace of dimension n_d for E_n. Define $n_d \times m_d$ matrix $H_{\mathbf{nm}}$ with its entries being

$$H_{nn_i,mm_j} = \langle n, n_i| H |m, m_j\rangle. \tag{15}$$

Consider the first order derivative to the entropy, we have $\alpha\alpha$

$$\begin{aligned} \frac{dS(\rho_0)}{d\varepsilon} &= \sum_n \int_0^\infty E_n(E_n + t)^{-2} Tr H_{\mathbf{nn}} dt - \sum_n Tr H_{\mathbf{nn}} \log E_n \\ &= -\sum_n Tr H_{\mathbf{nn}} \log E_n. \end{aligned} \tag{16}$$

Since $TrH_{\mathbf{nn}} = \sum_{i=1}^{n_d} \langle n, n_i| H |n, n_i\rangle$ is an invariant in the subspace, the first order perturbation to the entropy can be written as $-\sum_k H_{kk} \log E_k$, where k is the unified label for all the distinct eigenvectors (for some $k' \neq k$, we may have $E_{k'} = E_k$). Thus the degenerate of the eigenvalues will not affect the expression of the first order perturbation of the entropy. With the notation of $H_{\mathbf{nm}}$, it follows the second order derivative to the entropy

$$\frac{d^2 S(\rho_0)}{d\varepsilon^2} = -\sum_n \frac{Tr[H_{\mathbf{nn}} H_{\mathbf{nn}}^T]}{E_n} - 2 \sum_{n,m\neq n} \frac{Tr[H_{\mathbf{nm}} H_{\mathbf{nm}}^T]}{E_n - E_m} \log E_n \tag{17}$$

where $Tr[H_{\mathbf{nn}} H_{\mathbf{nn}}^T] = Tr[H_{\mathbf{nn}} H_{\mathbf{nn}}^*] = \sum_{i,j} |H_{nn_i,nn_j}|^2$ is the summation of the absolute square of all entries of the matrix $H_{\mathbf{nn}}$,not the summation of the absolute square of diagonal entries of the matrix $H_{\mathbf{nn}}$.

3.2 Perturbation to the two-mode thermal state

Let $\rho_T = (1-v)\sum_{n=0}^{\infty} v^n |n\rangle\langle n|$ be single-mode thermal state, the direct product of ρ_T with itself will result a two-mode $\rho_2 = \rho_T \times \rho_T$. The characteristic function of ρ_2 is $\chi_2(\mu_1,\mu_2) = \exp[-(N+\frac{1}{2})(|\mu_1|^2+|\mu_2|^2)]$. We consider the perturbed characteristic function $\chi(\mu_1,\mu_2) = \chi_2(\mu_1,\mu_2)[1+\varepsilon(\alpha\mu_1\mu_2+\alpha^*\mu_1^*\mu_2^*)]$. The perturbed density operator is $\rho = \rho_2 + \varepsilon H$, with

$$H = (1-v)^2(\alpha^* a_1^\dagger a_2^\dagger \rho_2 + \alpha\rho_2 a_1 a_2), \tag{18}$$

where $a_i^\dagger$ and a_i are the creation and annihilation operator for the two modes, respectively. The state $\rho_2 = (1-v)^2\sum_{n=0}^{\infty}\sum_{j=0}^{n} v^n |j,n-j\rangle\langle j,n-j|$. For any given $n>0$, the state is $(n+1)$-fold degenerate. In the eigenbasis of ρ_2, the entries of matrix $H_{\mathbf{nm}}$ are

$$\begin{aligned}\langle j,n-j|H|k,m-k\rangle &= (1-v)^2[\alpha^*\delta_{j,k+1}\delta_{n,m+2}E_{n-2}\sqrt{j(n-j)} \\ &\quad +\alpha\delta_{j,k-1}\delta_{n,m-2}E_n\sqrt{(j+1)(n-j+1)}],\end{aligned} \tag{19}$$

where $E_n = (1-v)^2 v^n$ is the eigenvalue of ρ_2. Clearly, $H_{\mathbf{nn}}$ now is a zero matrix, so that $TrH_{\mathbf{nn}} = Tr[H_{\mathbf{nn}}H_{\mathbf{nn}}^T] = 0$. We only need to evaluate the second term of Eq. (17). We have

$$\begin{aligned}\sum_{n,m\neq n}\frac{Tr[H_{\mathbf{nm}}H_{\mathbf{nm}}^T]}{E_n-E_m}\log E_n &= (1-v)^4|\alpha|^2\sum_n[\frac{E_{n-2}^2}{E_n-E_{n-2}}\sum_{j=0}^{n} j(n-j) \\ &\quad +\frac{E_n^2}{E_n-E_{n+2}}\sum_{j=0}^{n}(j+1)(n-j+1)]\log v^n \\ &= -\frac{2|\alpha|^2}{1+v}\log\frac{1}{v}.\end{aligned} \tag{20}$$

Thus the entropy of the perturbed state will be

$$S(\rho) = 2S(\rho_T) - \frac{\varepsilon^2|\alpha|^2}{1+v}\log\frac{1}{v} + o(\varepsilon^2). \tag{21}$$

4 Density operator expansion

In the calculation of the coherent information, even if we assume that the input state undergo a simple form perturbation $\rho = \rho_0 + \varepsilon H$, the output state $\mathcal{E}(\rho)$ and the combined output state $(\mathcal{I}\otimes\mathcal{E}\ )|\Psi\rangle\langle\Psi|$ may have a more complicated perturbation structures by the application of channel map $\mathcal{E}$ and the purification from ρ to $|\Psi\rangle$. So that we need to consider a more generic form of perturbation:

$$\rho = \rho_0 + \varepsilon H^{(1)} + \varepsilon^2 H^{(2)} + \varepsilon^3 H^{(3)} + \cdots. \tag{22}$$

It is reasonable to require that $TrH^{(n)} = 0$ is true for each n. The entropy perturbation can be obtained in due course, which is

$$\begin{aligned}S(\rho) &= S(\rho_0) - \sum_{n=1}^{\infty}\varepsilon^n Tr[H^{(n)}\log\rho_0] - \sum_{n=2}^{\infty}\varepsilon^n\sum_{j=2}^{n}(-1)^j\sum_{i_1 i_2\cdots i_j}\int_0^\infty t(\rho_0+t)^{-1}H^{(i_1)}(\rho_0+t)^{-1} \\ &\quad \times H^{(i_2)}(\rho_0+t)^{-1}\cdots H^{(i_j)}(\rho_0+t)^{-1}\delta_{i_1+i_2+\cdots+i_j,n}.\end{aligned} \tag{23}$$

We may express the second and the third order derivatives of the entropy in more explicit forms:

$$\begin{aligned}\frac{1}{2!}\frac{d^2S(\rho_0)}{d\varepsilon^2} &= -Tr\int_0^\infty t(\rho_0+t)^{-1}H^{(1)}(\rho_0+t)^{-1}H^{(1)}(\rho_0+t)^{-1}dt \\ &\quad -Tr[H^{(2)}\log\rho_0],\end{aligned} \tag{24}$$

$$\begin{aligned}\frac{1}{3!}\frac{d^3S(\rho_0)}{d\varepsilon^3} &= Tr\int_0^\infty t(\rho_0+t)^{-1}[H^{(1)}(\rho_0+t)^{-1}]^3 dt \\ &\quad -2Tr\int_0^\infty t(\rho_0+t)^{-1}H^{(1)}(\rho_0+t)^{-1}H^{(2)}(\rho_0+t)^{-1}dt \\ &\quad -Tr[H^{(3)}\log\rho_0].\end{aligned} \tag{25}$$

To verify the entropy expansion formula, we consider the displacement of thermal state, $\rho_d = D(\varepsilon\alpha)\rho_T D^\dagger(\varepsilon\alpha)$. The characteristic function of the state is $\chi_d(\mu) = Tr[\rho_d D(\mu)] = Tr[\rho_T D^\dagger(\varepsilon\alpha)D(\mu)D(\varepsilon\alpha)] = \chi_T(\mu)\exp[\varepsilon(\alpha^*\mu - \alpha\mu^*)]$. Since the displacement operator is unitary, the entropy will not be changed by the displacement operation. Thus $S(\rho_d) = S(\rho_T)$, the entropy $S(\rho_d)$ is not a function of ε. If we expand the entropy of ρ_d with respect to ε, then the perturbation up to any order should be zero. Expanding with respect to ε, the characteristic function is

$$\chi_d(\mu) = \chi_T(\mu)[1 + \varepsilon(\alpha^*\mu - \alpha\mu^*) + \frac{1}{2!}\varepsilon^2(\alpha^*\mu - \alpha\mu^*)^2 + \cdots]. \tag{26}$$

The state is $\rho_d = \rho_T + \varepsilon H^{(1)} + \varepsilon^2 H^{(2)} + \cdots$, with

$$H^{(2)} = \frac{1}{2!}(1-v)^2[\alpha^2 a^{\dagger 2}\rho_T + \rho_T \alpha^{*2} a^2 + 2|\alpha|^2 a^\dagger \rho_T a] - (1-v)|\alpha|^2 \rho_T. \tag{27}$$

The $H^{(1)}$ term has been treated in the former section, which give rise to the first term of the right hand side of Eq. (24) the value $2|\alpha|^2 \log v$. And by direct calculation we have

$$-Tr[H^{(2)}\log\rho_0] = -2|\alpha|^2 \log v. \tag{28}$$

So $\frac{d^2 S(\rho_0)}{d\varepsilon^2} = 0$. The first and the third derivatives of the entropy should be 0 considering the symmetry of the system.

5 Discussion and Conclusion

In the examples presented, we obtain the density operator perturbation via the expansion of the characteristic function for continuous variable systems. This has some merits. First of all, since the characteristic function is a c-number function, its expansion is simply Taylor expansion. We do not consider the Laurent expansion of the complex function since for any state we have $\chi(0) = 1$. The characteristic function is defined as $\chi(\mu) = Tr[\rho D(\mu)]$, thus $\chi(0) = Tr[\rho D(0)] = Tr[\rho] = 1$. Secondly, we expand the characteristic function as $\chi(\mu) = \chi_0(\mu)[1 + \sum_{n=1}^{\infty}\varepsilon^n \sum_{i=0}^{n} c_{i,n-i}\mu^i\mu^{*j}]$ for the single-mode system (the multi-mode expansion can be obtained in due course). The unperturbed characteristic function $\chi_0(\mu)$ is reserved as an integral nuclear for each order of perturbations. Thus the $n-$th perturbation $H^{(n)} = \int \frac{d^2\mu}{\pi}\chi_0(\mu)\sum_{i=0}^{n} c_{i,n-i}\mu^i\mu^{*j}D(-\mu)$ can be obtained with the difficulty of non-integrable. This form of expansion also implies that $Tr[H^{(n)}] = 0$, which is not apparent at the first sight when we write down, for example, $H^{(2)}$ in Eq. (27), although it can be proved by simple calculation.

One of the obstacle that may be encountered in the entropy perturbation calculation is the 0 eigenvalues of the unperturbed system. For instance, we consider the perturbation to a pure state, the unperturbed eigenvalues are 0 and 1. This can be partially overcome by decomposing the perturbation matrix H as diagonal and off-diagonal part according to the eigensystem of the unperturbed density matrix ρ_0. Suppose $\rho = \rho_0 + \varepsilon(H_0 + H')$, with H_0 being diagonal and H' being off-diagonal in the eigenbasis of ρ_0. So ρ_0 and H_0 can be diagonalized simultaneously. Thus the perturbed state can be written as $\rho = \rho_0' + \varepsilon H'$ with a new expansion base state $\rho_0' = \rho_0 + \varepsilon H_0$. Usually the eigenvalues of ρ_0' will differ from 0.

We have derived the entropy perturbation formula for degenerate and non-degenerate system. Up to any give order of perturbation of the density operator, the entropy perturbation was written in a concise form via operator integral, the integral then can be evaluated in the eigenbasis of the unperturbed density operator of the system.

Appendix A: The n-th order derivative of entropy

$\frac{d^n S(\rho_0)}{d\varepsilon^n} == P_3 + P_4$, with

$$
\begin{aligned}
P_3 &= -\lim_{\varepsilon\to 0}\frac{1}{\varepsilon^n}\sum_{l=0}^{n} Tr\rho_0\log(\rho_0 t+l\varepsilon)\binom{l}{n}(-1)^{n-l} \\
&= -\lim_{\varepsilon\to 0}\frac{(-1)^n}{\varepsilon^n}\sum_{l=0}^{n}(-1)^l\binom{l}{n}Tr\rho_0\int_0^\infty \frac{-dt}{\rho_0+l\varepsilon+t} \\
&= \lim_{\varepsilon\to 0}\frac{(-1)^n}{\varepsilon^n}\sum_{l=0}^{n}(-1)^l\binom{l}{n}Tr\rho_0\int_0^\infty \frac{dt}{t}\sum_{m=0}^{\infty}(-\frac{\rho_0+l\varepsilon H}{t})^m \\
&= \lim_{\varepsilon\to 0}\frac{(-1)^n}{\varepsilon^n}\sum_{l=0}^{n}(-1)^l\binom{l}{n}Tr\rho_0\int_0^\infty \frac{dt}{t}\sum_{m=n}^{\infty}\sum_{i_1,\cdots i_n}(-\frac{\rho_0}{t})^{i_1}\frac{l\varepsilon H}{t}\cdots(-\frac{\rho_0}{t})^{i_n}\frac{l\varepsilon H}{t}(-\frac{\rho_0}{t})^{m-n-\sum_{j=0}^{n} i_j}(-1)^n \\
&= \sum_{l=0}^{n}(-1)^l\binom{l}{n}l^n\int_0^\infty Tr\rho_0(\rho_0+t)^{-1}[H(\rho_0+t)^{-1}]^n dt \\
&= (-1)^n n!\int_0^\infty Tr\rho_0(\rho_0+t)^{-1}[H(\rho_0+t)^{-1}]^n dt.
\end{aligned}
$$

The last equation cames from the identity $\sum_{l=0}^{n}(-1)^l\binom{l}{n}l^n=(-1)^n n!$. In the fourth equation we have used the fact that $\sum_{l=0}^{n}(-1)^l\binom{l}{n}l^m=0$ for all $m<n$. We now prove this two results. Assuming $g(x)=(1-x)^n=\sum_{l=0}^{n}(-1)^l\binom{l}{n}x^l$, let $f_m(x)=\left[x\frac{d}{dx}\right]^m g(x)=\sum_{l=0}^{n}(-1)^l\binom{l}{n}l^m x^l$, then $f_m(x)=\sum_{k=1}^{m}c_k^{(m)}x^k\frac{d^k g(x)}{dx^k}$, where $c_k^{(m)}$ is the coefficient which obey the recursive relation $c_k^{(m+1)}=kc_k^{(m)}+c_{k-1}^{(m)}$. We always have $c_m^{(m)}=1$. Note that $\frac{d^k g(0)}{dx^k}=0$, for all $k<n$, and $\frac{d^k g(0)}{dx^k}=(-1)^n n!$, for $k=n$. Thus we have $\sum_{l=0}^{n}(-1)^l\binom{l}{n}l^n=f_n(1)=(-1)^n n!$ and $\sum_{l=0}^{n}(-1)^l\binom{l}{n}l^m=f_m(1)=0$ for all $m<n$.

P_4 can be obtained in the very similar way.

Appendix B: The third and fourth order off-diagonal perturbation

When the perturbation is off-diagonal in the eigenbasis of the unperturbed state, we have $H_{nn}=0$. The contribution to the third order perturbation should be

$$Q_3=\int_0^\infty Tr\{t(\rho_0+t)^{-1}[H(\rho_0+t)^{-1}]^3\}dt.$$

Evaluating in the basis of ρ_0, we have

$$Q_3=\sum_{n,m,k}\int_0^\infty \frac{tH_{nm}H_{mk}H_{kn}}{(E_n+t)^2(E_m+t)(E_k+t)}dt.$$

The summation should be taken for the case that n,m and k are all different since $H_{nn}=0$. After integrating and considering the permutation symmetry, we have

$$Q_3=\sum_{n<m<k}\frac{2Re(H_{nm}H_{mk}H_{kn})}{E_m-E_k}[\frac{\log(E_n/E_k)}{(E_n-E_k)}-\frac{\log(E_n/E_m)}{E_n-E_m}],$$

The contribution to the fourth order perturbation is

$$Q_4=\sum_{n,m,l,k}\int_0^\infty \frac{tH_{nm}H_{ml}H_{lk}H_{kn}}{(E_n+t)^2(E_m+t)(E_l+t)(E_k+t)}dt.$$

When all n,m,l,k are different with each other, the integral will be

$$
\begin{aligned}
Q_{41} = &\sum_{n<m<l<k} 2Re(H_{nm}H_{ml}H_{lk}H_{kn}+H_{nm}H_{ml}H_{lk}H_{kn}+H_{nm}H_{ml}H_{lk}H_{kn}) \\
&[\frac{\log(E_m/E_n)}{(E_m-E_n)(E_m-E_l)(E_m-E_k)}+\frac{\log(E_l/E_n)}{(E_l-E_n)(E_l-E_m)(E_l-E_k)} \\
&+\frac{\log(E_k/E_n)}{(E_k-E_n)(E_k-E_m)(E_k-E_l)}],
\end{aligned}
$$

where permutation symmetry are considered. When two of n, m, l, k are equal, that is (i) $n = l \neq m \neq k$ and (ii) $m = k \neq n \neq l$, the integral will be

$$Q_{42} = \sum_{n,m,k} \int_0^\infty \frac{t\,|H_{nm}H_{nk}|^2}{(E_n+t)^3(E_m+t)(E_k+t)}dt + \sum_{n,l,m} \int_0^\infty \frac{t\,|H_{mn}H_{ml}|^2}{(E_n+t)^2(E_m+t)^2(E_l+t)}dt.$$

which is

$$\begin{aligned} Q_{42} &= \sum_{n<m<k} (|H_{nm}H_{nk}|^2 + |H_{mn}H_{mk}|^2 + |H_{kn}H_{km}|^2) \\ &\quad [\frac{1}{E_n(E_n-E_m)(E_n-E_k)} + \frac{\log(E_m/E_n)}{(E_m-E_n)^2(E_m-E_k)} + \frac{\log(E_k/E_n)}{(E_k-E_n)^2(E_k-E_m)}]. \end{aligned}$$

When $n = l$ and $m = k$, we have the integral

$$Q_{43} = \sum_{n,m} \int_0^\infty \frac{t\,|H_{nm}|^4}{(E_n+t)^3(E_m+t)^2}dt,$$

which is

$$Q_{43} = \sum_{n<m} |H_{nm}|^4 [\frac{1}{2(E_n-E_m)^2}(\frac{1}{E_n}+\frac{1}{E_m}) - \frac{1}{(E_n-E_m)^3}\log\frac{E_n}{E_m}].$$

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